Quantum separability, time reversal and canonical decompositions

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Abstract

We propose an interpretation of quantum separability based on a physical principle: local time reversal. It immediately leads to a simple characterization of separable quantum states that reproduces results known to hold for binary composite systems and which thereby is complete for low dimensions. We then describe a constructive algorithm for finding the canonical decomposition of separable and non separable mixed states of dimensions 2x2 and 2x3.

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Entanglement, inseparability and nonlocality are some of the most genuine quantum concepts. As it has been pointed out, we still lack a complete classification of quantum states in local and non-local ones [1], or more precisely we still lack the complete understanding of non-locality. Thus, while for pure states it is well established since long ago that the non-local character of the composite system is revealed in different but equivalent ways, the situation is drastically different for mixed states. For example, for pure states the violation of some kind of Bell inequalities [2], or the demonstration that no local hidden variable models can account for the correlations between the observables in each subsystem, are equivalent definitions of non-locality. But for mixed states, described by density matrices, such equivalences fade away. Consider a composite quantum system described by a density matrix ρ in the Hilbert space $\mathcal{H}_a \otimes \mathcal{H}_b$. In the frame set by the concepts of our starting sentence, product or factorizable states are the simplest possible. They are of the form $\rho_p = \rho_a \otimes \rho_b$, i.e. for them, and only for them, the description of the two isolated subsystems is equivalent to the description of the composite system. Recalling that subsystems are described by the reduced density matrices obtained via partial tracing: $\rho_a = Tr_b \rho$ ($\rho_b = Tr_a \rho$), a density matrix corresponds to a product or factorizable state if and only if

$$\rho = Tr_b \rho \otimes Tr_a \rho \iff \rho = \rho_p \tag{1}$$

Also their index of correlation defined in terms of von Neumann entropies of the system and subsystems,

$$I_c = Tr \rho \ln \rho - Tr \rho_a \ln \rho_a - Tr \rho_b \ln \rho_b \tag{2}$$

vanishes, and this happens only for them [3]. Their subsystems are uncorrelated. Any state which is not a product state presents some kind of correlation. They are called correlated states. Quantum mechanics has taught us that there is a hierarchy of correlations, and the physics in the different ranks is different. The simplest correlated systems are the classically correlated or separable systems. Their density matrices can always be written in the form:

$$\rho_s = \sum_i p_i \rho_{ai} \otimes \rho_{bi}; \quad 1 \geq p_i \geq 0; \ \sum_i p_i = 1 \tag{3}$$

i.e. as a mixture of product states. Their characterization is notoriously difficult. Thus, given a density matrix which is known to describe a separable system no algorithm for decomposing it according to eq. (3) is known; besides, the decomposition is not unique. In fact, only very recently Peres and the Horodecki family [4,5] have obtained a mathematical characterization of these states, at least when the dimension of the composite Hilbert space is 2×2 or 2×3. For these cases the necessary and sufficient condition for separability is that the matrix obtained by partially transposing the density matrix ρ is still a density matrix, i.e. hermitian, with unity trace and non-negative eigenvalues

$$\rho^{T_b} = (\rho^{T_a})^* \geq 0 \iff \rho = \rho_s \tag{4}$$

For composite systems described by Hilbert spaces of higher dimensions, the positivity condition of ρ^{T_b} is only a necessary one for separability [5]. Following the hierarchy of correlations, we find the states that are no longer separable (or classically correlated), i.e. $\rho \neq \rho_s$. These states are called "EPR-states" [6], "inseparable", "non-local", and

sometimes "entangled" or simply "quantum-correlated" to emphasize that their correlations are not strictly classical anymore, though often these labels do not refer to exactly the same states. This confusion reflects the need of a further subclassification of the inseparable states according to whether they admit local hidden variables, whether they violate some kind of Bell inequality [7,8], etc..

The aim of this Letter is threefold. Firstly, we give a physical interpretation of the mathematical characterization of separability (Eq. (4)). Secondly, we provide a constructive "canonical" algorithm for decomposing any separable matrix (of dimension ≤ 6) into a very small finite incoherent sum of product vectors. Finally, we show that a similar decomposition holds for inseparable states, with the signature of non-separability being expressed by some non-positive weights in the canonical decomposition.

Let us first analyze the problem of separability from a physical point of view. We start by considering symmetry transformations in the Hilbert space of each subsystem. We limit ourselves in this paper to just binary composite systems , i.e. $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$. Wigner's theorem tells us that every symmetry transformation should always be implemented by a unitary (U) or antiunitary (A) matrix. The direct product of unitary matrices $U_a \otimes U_b$ (or antiunitary matrices $A_a \otimes A_b$) is a unitary (or antiunitary) matrix in the Hilbert space of the composite system $\mathcal{H}$, and one can give an unambiguous definition of how such a transformation acts on any ket $|\Psi\rangle \in \mathcal{H}$. However, the combination of a unitary and an antiunitary transformation $U_a \otimes A_b$ (or $A_a \otimes U_b$) results in a transformation which is neither unitary nor antiunitary in $\mathcal{H}$, whose action on a general ket of the composite system $|\Psi\rangle \in \mathcal{H}$, furthermore, cannot be properly defined. However, its action on a product ket $|e\rangle \otimes |f\rangle \equiv |e, f\rangle$, (where $|e\rangle \in \mathcal{H}_a$ and $|f\rangle \in \mathcal{H}_b$) is, but for a phase ambiguity, well defined. Thus, the action of combined transformation of the type $U_a \otimes A_b$ on projectors corresponding to pure product state is well defined without any ambiguity. As a separable state can always be rewritten as a statistical mixture of product vectors:

$$\rho_s = \sum_i p_i(|e_i\rangle\langle e_i| \otimes |f_i\rangle\langle f_i|);\ 1 \geq p_i \geq 0;\ \sum_i p_i = 1 \tag{5}$$

it is clear that under the combined transformation $U_a \otimes A_b$ (or $A_a \otimes U_b$) ρ_s transforms into:

$$\rho_s \to \rho_s^{'} = \sum_i p_i \left(|e_i^{'}\rangle\langle e_i^{'}| \otimes |f_i^{'}\rangle\langle f_i^{'}|\right) \tag{6}$$

where $|e_i^{'}\rangle \equiv U_a|e_i\rangle \in \mathcal{H}_a$; $|f_i^{'}\rangle \equiv A_b|f_i\rangle \in \mathcal{H}_b$. Therefore, $\rho_s^{'}$ describes also a physical state so that $\rho_s^{'}$ is a positive defined hermitian matrix (with normalized trace). This is what characterizes separable states: that any local symmetry transformation, which obviously transforms local physical states into local physical states, also transforms the global physical state into another physical state. (Here and in what follows "local" means that it refers to the subsystems).

There exists only one independent antiunitary symmetry and its physical meaning is well known: time reversal. Any other antiunitary transformation can be expressed in terms of time reversal (as the product of a unitary matrix times time reversal). We are thus proposing that quantum separability of composite systems implies the lack of correlation between the time arrows of their subsystems. In other words: for separable states, the state one obtains by reversing time in one of its subsystems is also a physical state. Loosely speaking,

systems which are classically correlated (separable) do not have memory of a unique time direction in the sense "EPR" correlated states have, and they are thus compatible with a time evolution which factorizes into the product of two opposed time evolutions. Changing the time direction in only one of the subsystems but not in both leads to a physical state since their time arrows are uncorrelated.

We can define now the "separability" operator as the simplest possible transformation of this type:

$$S \equiv I_a \otimes K_b \tag{7}$$

where I_a stands for the identity acting in the first subsystem $\mathcal{H}_a$ and K_b is the complex conjugation operator acting in $\mathcal{H}_b$ [9]. It is straightforward to check that in the Hilbert-Schmidt basis [10] of 2×2 composite systems:

$$S\rho S = \rho^{T_b} \tag{8}$$

for any ρ, whether it is separable or not, in spite of the fact that the action of S on a general $|\Psi\rangle \in \mathcal{H}$ cannot be properly defined. (This feature of being able to define a transformation on density matrices which one cannot define on kets is known for some nonunitary transformations, as e.g. a decohering time-evolution). Finally, as local time reversal is locally unitarily equivalent to expression (7), eqs.(4) and (8) state that for 2x2 composite systems a state is separable if and only if it does not correlate local time flows. The same holds for a 2x3 composite system.

Let us go to the second point of our Letter, the "canonical" decomposition of a separable density matrix. Until very recently it was not known whether one could always find a finite incoherent sum of pure product states for any separable ρ_s. P. Horodecki [11] and Vedral et al. [12] have shown that any separable state ρ_s can be decomposed into an incoherent sum of at most $N = (dim(\mathcal{H}_a) \times dim(\mathcal{H}_b))^2$ pure product states, although no algorithm for obtaining this decomposition seems to be known. We will limit ourselves here, again, to the simplest possible case, i.e. binary composite systems of dimensions $dim(\mathcal{H}_a) = dim(\mathcal{H}_b) = 2$. In such cases, any separable density matrix can be written as a statistical mixture of at most N=16 pure product states. Let us show here that one can do much better: indeed, any separable density matrix can be written as a convex combination of at most $N = 5$ pure product vectors. The whole proof of such a decomposition is based on the following theorems:

Theorem1 For any plane $\mathcal{P}_1$ in $\mathcal{C}^2 \otimes \mathcal{C}^2$ defined by two product states $|v_1\rangle$ and $|v_2\rangle$ (where $|v_i\rangle = |e_i\rangle \otimes |f_i\rangle$; $|e_i\rangle \in \mathcal{H}_a$ and $|f_i\rangle \in \mathcal{H}_b$) either all the states in this plane are product states, or there is no other product states in it.

Theorem2 There exist planes $\mathcal{P}_2$ in $\mathcal{C}^2 \otimes \mathcal{C}^2$ which contain only one product state.

Theorem 3 Any plane $\mathcal{P}_3$ in $\mathcal{C}^2 \otimes \mathcal{C}^2$ contains at least one product state.

The proofs of the theorems are simple. It is convenient to express, with the help of the $SU(2) \otimes SU(2)$ transformations, the planes defined by the theorems (denoted as $\mathcal{P}_1$,$\mathcal{P}_2$ and $\mathcal{P}_3$) as:

$$\mathcal{P}_1(\alpha_1, \beta_1) \equiv \alpha_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta_1 \begin{pmatrix} \cos A \\ e^{iB} \sin A \end{pmatrix} \otimes \begin{pmatrix} \cos C \\ e^{iD} \sin C \end{pmatrix} \tag{9}$$

with $0 \leq A, C \leq \pi/2$; $0 \leq B, D < 2\pi$, and $\alpha_1, \beta_1 \in \mathcal{C}$.

$$\mathcal{P}_2(\alpha_2, \beta_2) \equiv \alpha_2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta_2 \begin{pmatrix} 0 \\ cosA \\ e^{iC} \sin A \cos B \\ \sin A \sin B \end{pmatrix} \tag{10}$$

with $0 < A < \pi/2$; $0 \leq B < \pi/2$; $0 \leq C < 2\pi$, and $\alpha_2, \beta_2 \in \mathcal{C}$. Finally:

$$\mathcal{P}_3(\alpha_3, \beta_3) \equiv \alpha_3 \begin{pmatrix} \cos A \\ 0 \\ 0 \\ \sin A \end{pmatrix} + \beta_3 \begin{pmatrix} \sin A \cos B \\ \sin B \cos C \\ e^{iD} \sin B \sin C \\ -\cos A \cos B \end{pmatrix} \tag{11}$$

with $0 < A < \pi/2$; $0 \leq B, C \leq \pi/2$; $0 \leq D < 2\pi$, and $\alpha_3, \beta_3 \in \mathcal{C}$. There are further conditions that have to be imposed in Eq.(11) to ensure that the second state is not a product state. Solving for the values of α_i and β_i allows to prove the theorems. A consequence of the above theorems is the following corollary:

Corollary If ρ has rank 2 and is separable it can always be written as a statistical mixture of two pure product states, and thus ρ^{T_b} is also of rank 2.

Consider now a separable state ρ_s such that both itself and its partially transposed matrix are of rank 4,

$$r(\rho_s) = r(\rho_s^{T_b}) = 4 \tag{12}$$

(All other cases are subcases of this one, as we shall see immediately). Define now

$$\rho(p) \equiv \frac{1}{1-p}(\rho_s - p|e_1, f_1\rangle\langle e_1, f_1|); \;\; 0 < p < 1 \tag{13}$$

where $|e_1\rangle \in \mathcal{H}_a$ and $|f_1\rangle \in \mathcal{H}_b$ are completely arbitrary kets. For p small enough both ρ and ρ^{T_b}

$$\rho^{T_b}(p) \equiv \frac{1}{1-p}(\rho_s^{T_b} - p|e_1, f_1^*\rangle\langle e_1, f_1^*|); \;\; 0 < p < 1 \tag{14}$$

are positive, and therefore, due to eq.(4), separable. Let us denote by p_1 the smallest value for which a zero eigenvalue appears in $\rho(p)$ or $\rho^{T_b}(p)$. Let us assume that for p_1 one eigenvalue of $\rho(p)$ is equal to zero, i.e. $r(\rho(p_1)) = 3$ and $r(\rho^{T_b}(p_1)) = 4$ (the same argument holds for the opposite case). Consider now a new pure product vector state belonging to the range of $\rho(p_1)$; $|e_2, f_2\rangle \in \mathcal{R}(\rho(p_1))$ and define a new density matrix:

$$\bar{\rho}(p) \equiv \frac{1}{1-p}(\rho(p_1) - p|e_2, f_2\rangle\langle e_2, f_2|); \;\; 0 < p < 1. \tag{15}$$

As before, for p small enough, both $\bar{\rho}(p)$ and $\bar{\rho}^{T_b}(p)$ are non-negative and thus separable. Let us denote by p_2 the smallest value of p for which either $\bar{\rho}(p)$ or $\bar{\rho}^{T_b}(p)$ develop a new vanishing eigenvalue. It cannot be $\bar{\rho}(p)$ unless, because of the corollary, $\bar{\rho}^{T_b}(p)$ develops

simultaneously two vanishing eigenvalues. Therefore, it is in general $\bar{\rho}^{T_b}(p)$ which will develop a new vanishing eigenvalue, so that

$$r(\bar{\rho}(p_2)) = r(\bar{\rho}^{T_b}(p_2)) = 3. \tag{16}$$

As $\bar{\rho}(p_2)$ has a decomposition of the type of eq.(5) with at least three terms, and $\bar{\rho}^{T_b}(p_2)$ has the corresponding partially transposed one, there exist always a product state satisfying [11] : $|e_3, f_3\rangle \in \mathcal{R}(\bar{\rho}(p_2))$ and $|e_3, f_3^\star\rangle \in \mathcal{R}(\bar{\rho}^{T_b}(p_2))$ where the following identity:

$$(|\phi\rangle\langle\phi|)^T = (|\phi\rangle\langle\phi|)^\star \tag{17}$$

and some results by Hughston et al. [13] have been used. Define now:

$$\tilde{\rho}(p) \equiv \frac{1}{1-p}(\bar{\rho}(p_2) - p|e_3, f_3\rangle\langle e_3, f_3|); \ \ 0 < p < 1. \tag{18}$$

It is clear from the above results that a p_3 exists such that:

$$r(\tilde{\rho}(p_3) \geq 0) = r(\tilde{\rho}^{T_b}(p_3) \geq 0) = 2 \tag{19}$$

Finally, from the corollary, we know that there exists always the following decomposition:

$$\begin{aligned} \tilde{\rho}(p_3) \equiv\ & p_4|e_4, f_4\rangle\langle e_4, f_4| \\ & + (1-p_4)|e_5, f_5\rangle\langle e_5, f_5|; \ \ 0 < p_4 < 1. \end{aligned} \tag{20}$$

And from there our final results follows immediately:

$$\begin{aligned} \rho_s = \ & p_1 P_1 + p_2(1-p_1)P_2 \\ & + p_3(1-p_2)(1-p_1)P_3 \\ & + p_4(1-p_3)(1-p_2)(1-p_1)P_4 \\ & + (1-p_4)(1-p_3)(1-p_2)(1-p_1)P_5 \end{aligned} \tag{21}$$

where $P_i \equiv |e_i, f_i\rangle\langle e_i, f_i|$ are projectors onto pure product states.

It is obvious that this decomposition is far from unique. It is also clear that often one can simplify the first two steps to one, i.e. go from expression (12) to expression (16) by subtracting only one single pure product state. This can always be done, by continuity, when for some $|e, f\rangle$ it happens that $r(\rho(p_1)) = 3$ and $r(\rho^{T_b}(p_1)) = 4$ and for others $r(\rho(p_1)) = 4$ and $r(\rho^{T_b}(p_1)) = 3$. We do not know, right now, whether it can always be done, i.e. if any separable density matrix can always be written as a statistical mixture of just N=4 pure product states.

Let us now discuss our third result. Recall that for $dim(\mathcal{H}) = 4$ a state has quantum correlations iff ρ^{T_b} has at least one negative eigenvalue:

$$inf\, \sigma(\rho^{T_b}) < 0 \Longleftrightarrow \rho = \rho_q \tag{22}$$

where $\sigma(\rho)$ means the spectrum of ρ and the subscript q means quantum correlated. Let us prove now that there is only one negative eigenvalue. If there were two, one could always find,

according to our theorem, a product state $|e,f\rangle$ in the plane defined by the corresponding two eigenvectors, and for which obviously

$$\langle e,f|\rho_q^{T_b}|e,f\rangle < 0. \tag{23}$$

But the above expression is equivalent, recalling the Hilbert-Schmidt decomposition, to

$$\langle e,f^\star|\rho_q|e,f^\star\rangle < 0, \tag{24}$$

which is impossible. Let us then define

$$\begin{aligned}\rho^{T_b}(p_1,p_2) \equiv \frac{1}{1+p_1+p_2}&(\rho_q^{T_b} + p_1|e_1,f_1\rangle\langle e_1,f_1| \\ &+ p_2|e_2,f_2\rangle\langle e_2,f_2|)\ , p_i \geq 0,\end{aligned} \tag{25}$$

where $|e_i,f_i\rangle$ are the two product states of the Schmidt decomposition of the negative eigenvalue eigenvector of $\rho_q^{T_b}$; $|n\rangle = c_1|e_1,f_1\rangle + c_2|e_2,f_2\rangle$. For some finite values of p_1 and p_2, $\bar{p}_1$ and $\bar{p}_2$, $r(\rho_q^{T_b}(\bar{p}_1,\bar{p}_2) \geq 0) = 3$. As $\rho_q(\bar{p}_1,\bar{p}_2) \geq 0$ the algorithm proceeds as before for the separable states. Thus

$$\begin{aligned}\rho_q = (1+\bar{p}_1+\bar{p}_2)\rho_s(4) &- \bar{p}_1|e_1,f_1^\star\rangle\langle e_1,f_1^\star| \\ &- \bar{p}_2|e_2,f_2^\star\rangle\langle e_2,f_2^\star|,\end{aligned} \tag{26}$$

where $\rho_s(4)$ is a statistical mixture of $N=4$ pure product states. Certainly, expression (26) is not a statistical mixture in the sense that two weights in the decomposition are negative, but that only means that ρ_q, which is a statistical mixture of pure states, is inseparable. Often one can find a decomposition of the type (26) but with only five terms, either having $\rho_s(3)$ or only one $\bar{p}$, but we do not know yet if this is always possible. Also, $\bar{p}_i$ are measures of the inseparability of the state, which, supplemented with an adequate minimization procedure, might lead to a faithful quantification of entanglement [14,15].

Finally, let us illustrate our procedure with a simple example. Consider a pair of spin-$\frac{1}{2}$ particles in an impure state consisting of a singlet fraction x and an isotropical mixture of the singlet and the triplet mixed in equal proportions [7]:

$$\begin{aligned}\rho_w = x|\Psi^-\rangle\langle\Psi^-| + \frac{(1-x)}{4}&(|\Psi^-\rangle\langle\Psi^-| \\ + |\Psi^+\rangle\langle\Psi^+| + |\Phi^+\rangle\langle\Phi^+| &+ |\Phi^-\rangle\langle\Phi^-|)\end{aligned} \tag{27}$$

where $0<x<1$, $|\Psi^\pm\rangle \equiv 1/\sqrt{2}(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$, and $|\Phi^\pm\rangle \equiv 1/\sqrt{2}(|\uparrow\uparrow\rangle \pm |\downarrow\downarrow\rangle)$. The condition of separability (eq. 4) shows that ρ_w is separable for $x \leq 1/3$ and inseparable otherwise. One simple decomposition by following the procedure we have indicated is given by:

$$\begin{array}{ll} p_1 = \frac{(1+3x)(1-x)}{4(1+x)} & ;\ |e_1,f_1\rangle = \binom{1}{0} \otimes \binom{0}{1} \\ p_2 = \frac{(1-3x)(1+x)^2}{(3+2x+3x^2)(1-x)} & ;\ |e_2,f_2\rangle = \binom{1}{0} \otimes \binom{1}{0} \\ p_3 = \frac{1}{3} & ;\ |e_3,f_3\rangle = \frac{1}{\sqrt{3x^2+1}}\binom{2x}{-\sqrt{1-x^2}} \otimes \frac{1}{\sqrt{2}}\binom{\sqrt{1+x}}{\sqrt{1-x}} \\ p_4 = \frac{1}{2} & ;\ |e_4,f_4\rangle = \frac{1}{\sqrt{3x^2+1}}\binom{2x}{e^{i\pi/3}\sqrt{1-x^2}} \otimes \frac{1}{\sqrt{2}}\binom{\sqrt{1+x}}{e^{-i2\pi/3}\sqrt{1-x}} \\ & \quad |e_5,f_5\rangle = |e_4\rangle^\star \otimes |f_4\rangle^\star \end{array} \tag{28}$$

which also holds when ρ_w is inseparable, in which case p_2 becomes negative. One can extend most of our results straightforwardly to $dim[\mathcal{H}]$=6, but not beyond, as Eq.(4) does not hold anymore.

To summarize, we propose to characterize separable states by their inability of correlating local time arrows. For low enough dimensions this characterization is complete. We have also shown that it is always possible to find a decomposition with at most five pure product states to express any separable density matrix (for $dim[\mathcal{H}] = 4$). Moreover, when the state is inseparable a similar decomposition with at most six pure product states holds, where one or two of them have now a negative weight. We believe our results are a step forward in the understanding of quantum (non)separability.

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